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Scattering Wave Functions at Bound State Poles

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Abstract

The normalisation relation between the bound and scattering S-state wave functions, extrapolated to the bound state pole, is derived from the Schrödinger equation. It is shown that, unlike previous work, the result does not depend on the details of the potential through the corresponding Jost function but is given uniquely in terms of the binding energy. The generalisations to higher partial waves and one-dimensional scattering are given.

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1 Introduction

It is demonstrated in standard quantum mechanics texts [1] that when a scattering wave function is extrapolated to negative energy to the position of a bound state then the result is proportional to the bound state wave function. This is achieved through the divergence at this energy of the coefficient of the exponentially decreasing function at large distances.

Much less interest has been placed on the relative normalisations of the scattering and bound state wave functions. Goldberger and Watson [2] and subsequently Joachain [3] have given a formal expression for this in terms of the Jost function and its derivative, which suggests that this quantity will in fact depend upon the form of the potential.

We have recently shown [4], using results from formal scattering theory, that the continuation of an S-state scattering wave function with real boundary conditions to a bound state pole actually only depends upon the bound state wave function and binding energy. This result is counter-intuitive in that a scattering wave is normalised by its asymptotic behaviour at large distances, whereas a bound state is normalised by an integral condition. It is the purpose of the present work to give a self-contained demonstration of this starting from the Schrödinger equation and our principal result, eq.(25), is to be found in §2. The generalisation of this to higher partial waves is outlined in §3, where the importance threshold kinematic factors in the extrapolation to the bound state is stressed.

The relationship to the Goldberger and Watson form is investigated in §4, where it is shown that, carried to its logical conclusion, their form would give an answer identical to ours at the bound state position. Their extrapolation is, however, less smooth as a function of energy and, as a consequence, less useful in practice.

The equivalent theorem for one-dimensional scattering is derived in §5 and some discussion of the usefulness of the results given in the conclusions of §6.

2 Derivation of the Theorem

We start by summarising the relevant results of potential scattering as given, for example, in refs.[5, 6].

Consider a particle of mass m moving with energy $E = k^2/2m$ and angular momentum ℓ in a real spherically symmetric potential $V(r)$. In units where $\hbar = 1$, the radial Schrödinger equation becomes

$$\frac{\mathrm{d}^2}{\mathrm{d}r^2}\,\psi_\ell(k,r) + \left(k^2 - \frac{\ell(\ell+1)}{r^2}\right)\psi_\ell(k,r) = U(r)\,\psi_\ell(k,r)\,, \tag{1}$$

with $U(r) = 2mV(r)$.

In order that the results of standard scattering theory apply, we assume that the potential satisfies the integrability condition

$$\int_0^\infty \mathrm{d}r\, r \mid V(r) \mid < \infty\,. \tag{2}$$

This requires that the potential be less singular than r^{-2} at short distances but decrease more rapidly than r^{-2} at large ones. For such a regular potential the bound state eigenvalues of eq.(1) are non-degenerate and finite in number [6].

The generalisation to higher partial waves will be given in §3, and here we shall only consider S-wave solutions for which the index $\ell = 0$ on the radial wave function will be suppressed.

The Jost solution $f(k,r)$ is determined by the asymptotic behaviour

$$f(k,r) \stackrel{r\to\infty}{\longrightarrow} \mathrm{e}^{ikr}\,. \tag{3}$$

With this boundary condition the radial Schrödinger equation (1) can be transformed into an integral equation and it is then straightforward to show by iteration that $f(k,r)$ is analytic in the half-plane $\mathrm{Im}\{k\} > 0$ and is continuous and bounded in $\mathrm{Im}\{k\} \geq 0$ for all values of $r \geq 0$ [6].

The value of this solution at $r = 0$ is the Jost function

$$F(k) \equiv f(k,0)\,, \tag{4}$$

and, unless this vanishes, the full wave function resulting from the Jost solution will be singular at the origin.

In the scattering region, k is real and positive, whereas for a bound state $k = i\alpha$, with $\alpha > 0$ in order that the bound state be normalisable. For any fixed value of r the scattering wave function $f(k, r)$ can be analytically continued in k to give the bound state wave function $f(i\alpha, r)$ normalised such that it behaves like $\mathrm{e}^{-\alpha r}$ at large distances.

A second independent solution of the Schrödinger equation is $f(-k, r)$, and it is easy to see from the integral form of the equation that for $\mathrm{Im}\{k\} \geq 0$

$$f(-k^*, r) = f(k, r)^* \,, \tag{5}$$

from which it follows that for the Jost function

$$F(-k^*) = F(k)^* \,. \tag{6}$$

For our purposes of continuing to the bound state pole, it is crucial to work with a real function. A physical radial wave function $v(k, r)$ must vanish at the origin and the real linear combination with this property is

$$v(k, r) = \frac{1}{2ik} \left[f(k, r)\, \mathrm{e}^{i\delta(k)} - f(-k, r)\, \mathrm{e}^{-i\delta(k)} \right] \,, \tag{7}$$

with the phase shift $\delta(k)$ and corresponding S-matrix defined by

$$S(k) = \frac{F(-k)}{F(k)} = \mathrm{e}^{2i\delta(k)} \,. \tag{8}$$

The function $v(k, r)$ is real, due to the symmetry property of the Jost function shown in eq.(6), and behaves asymptotically like

$$v(k, r) \sim \frac{1}{k} \sin(kr + \delta(k)) \,. \tag{9}$$

The bound state positions are determined by demanding that the wave function decrease at large r and be finite at the origin, and this is achieved if $F(i\alpha) = 0$. The corresponding S-matrix has a pole at this position and it is known that such poles are simple for a well-behaved potential satisfying eq.(2) [6].

For positive real values of k the norm of the S-matrix is, by eq.(6), unity. We may parametrise it in the vicinity of an isolated bound state pole as

$$S(k) \equiv \mathrm{e}^{2i\delta(k)} = \frac{[N\,G(k)]^2}{\alpha + ik}\,, \tag{10}$$

where N^2 is the residue at the pole. In the unitarised scattering length approximation $N^2 = 2\alpha$ and $[G(k)]^2 = (\alpha - ik)/2\alpha$, but in general $G(k)$ is an analytic function of k in the neighbourhood of $k = i\alpha$, with the condition that $G(i\alpha) = 1$.

Comparing the radial S-wave Schrödinger equations for the bound and scattering state wave functions, we have

$$\begin{aligned} u''(r) - \alpha^2 u(r) &= U(r)\,u(r) \\ v''(k,r) + k^2 v(k,r) &= U(r)\,v(k,r)\,, \end{aligned} \tag{11}$$

where $U(r)$ is a real function.

The boundary conditions at the origin are $u(0) = v(k,0) = 0$, whereas the large-r behaviour of the bound state wave function is taken to be

$$u(r) \quad \stackrel{r\to\infty}{\longrightarrow} \quad \mathrm{e}^{-\alpha r}\,, \tag{12}$$

while that of $v(k,r)$ is given by eq.(9). The reality of the potential, combined with that of the boundary conditions, ensures that for real k the functions $u(r)$ and $v(k,r)$ remain real for all values of r.

The wave function $v(k,r)$ can be analytically continued in k to the bound state at $k = i\alpha$, though care must be taken due to the singularity structure of the factor $\mathrm{e}^{i\delta(k)}$. This is more complicated than its square, the S-matrix, since it has a branch cut starting at the position of the bound state.

It follows from eq.(10) that at the bound state pole

$$\left[\sqrt{2\alpha(\alpha^2 + k^2)}\,v(k,r)\right]_{k=i\alpha} = -\left[\sqrt{\alpha + ik}\,\mathrm{e}^{i\delta(k)}\right]_{k=i\alpha} f(i\alpha, r) = -Nu(r)\,. \tag{13}$$

It remains to be shown that the constant N is determined uniquely by the normalisation of the bound state wave function.

Manipulation of the radial Schrödinger equations in eq.(11) leads to

$$\frac{\mathrm{d}}{\mathrm{d}r}\left[u'(r)v(k,r) - u(r)v'(k,r)\right] = (\alpha^2 + k^2)u(r)v(k,r)\,, \tag{14}$$

where prime indicates derivative with respect to r. Since the functions vanish at the origin, this can be integrated to give

$$u'(r)v(k,r) - u(r)v'(k,r) = (\alpha^2 + k^2)\int_0^r \mathrm{d}r' u(r')v(k,r')\,. \tag{15}$$

Both sides of this equation vanish when $r \to \infty$, reflecting the orthogonality of the scattering and bound state wave functions. To avoid a $0 = 0$ statement, introduce the combination

$$w(k,r) \equiv 2ik\sqrt{\alpha + ik}\, v(k,r)\,, \tag{16}$$

which, by eq.(13), has the limit at the pole

$$w(i\alpha, r) = N\, u(r)\,. \tag{17}$$

Differentiating the resulting

$$u'(r)w(k,r) - u(r)w'(k,r) = (\alpha^2 + k^2)\int_0^r \mathrm{d}r' u(r')w(k,r') \tag{18}$$

with respect to k leads to

$$u'(r)\dot{w}(k,r) - u(r)\dot{w}'(k,r) = \int_0^r \mathrm{d}r' u(r')\left[(\alpha^2 + k^2)\dot{w}(k,r') + 2kw(k,r')\right]\,, \tag{19}$$

where derivatives with respect to k have been indicated by dots.

After taking first the limit $k \to i\alpha$ and then $r \to \infty$, the first term in the integrand vanishes because of the explicit $(\alpha^2 + k^2)$ factor, and so the right hand side of eq.(19) becomes

$$-2iN\alpha\int_0^\infty dr\, u^2(r)\,. \tag{20}$$

On the other hand, from the ansatz of eq.(10), in the vicinity of the pole

$$\begin{aligned} w(k,r) &= N\,G(k)\,f(k,r) - \frac{(\alpha + ik)}{N\,G(k)}\,f(-k,r)\,, \\ \dot{w}(k,r) &= N\,\dot{G}(k)\,f(k,r) + N\,G(k)\,\dot{f}(k,r) - \frac{i}{N\,G(k)}\,f(-k,r) \\ &\quad + \frac{(\alpha + ik)}{N\,G(k)}\,\dot{f}(-k,r) + \frac{(\alpha + ik)}{N\,G(k)^2}\,\dot{G}(k)\,f(-k,r)\,. \end{aligned} \tag{21}$$

Thus, since $G(i\alpha) = 1$ at the pole,

$$w(i\alpha, r) = N\, f(i\alpha, r) \stackrel{r\to\infty}{\longrightarrow} N\, \mathrm{e}^{-\alpha r}\,, \tag{22}$$

$$\dot{w}(i\alpha, r) = N\, \dot{G}(i\alpha)\, f(i\alpha, r) + N\, \dot{f}(i\alpha, r) - \frac{i}{N}\, f(-i\alpha, r)$$

$$\stackrel{r\to\infty}{\longrightarrow} -\frac{i}{N}\, \mathrm{e}^{+\alpha r}\,. \tag{23}$$

Since the bound state wave function decreases exponentially, the only surviving contributions to the left hand side of eq.(19) at large r originate from the term proportional to $f(-i\alpha, r)$ in eq.(23), yielding a value of $-2i\alpha/N$.

Equating the two sides of eq.(19), leads to the condition that

$$1 = N^2 \int_0^\infty \mathrm{d}r\, u^2(r)\,, \tag{24}$$

so that N is indeed the normalisation constant of the bound state wave function.

Rewriting the result in terms of a normalised radial bound state wave function $u_\alpha(r) = Nu(r)$, we see that the scattering wave function $v(k, r)$ is related to $u_\alpha(r)$ at the pole $k = i\alpha$ through

$$\lim_{k\to i\alpha} \left\{ \sqrt{2\alpha(\alpha^2 + k^2)}\, v(k, r) \right\} = -u_\alpha(r)\,, \tag{25}$$

and this is the principal result of this work.

It should be noted that, in contrast to the result given in ref.[3], the constant of proportionality in this relation is independent of the form of the potential and of the Jost function. Note also that, since a particular bound state is not specified, eq.(25) is valid at <u>all</u> bound state poles.

3 Higher partial waves

For higher ℓ-values the discussion given in §2 can be repeated with only minor changes. The Jost solutions of eq.(3) are determined by the asymptotic behaviour [6]

$$f_\ell(\pm k, r) \stackrel{r\to\infty}{\longrightarrow} \mathrm{e}^{i\pi\ell/2}\mathrm{e}^{\pm ikr}\,, \tag{26}$$

and the Jost functions defined as

$$F_\ell(\pm k) = \lim_{r\to 0}\left\{\frac{(\mp kr)^\ell}{(2\ell+1)!!}\, f_\ell(\pm k, r)\right\}\,. \tag{27}$$

The two Jost solutions are related for real k by

$$f_\ell(-k, r) = (-1)^\ell\, [f_\ell(k, r)]^*\,, \tag{28}$$

and similarly for the Jost functions.

The physical radial wave function $v_\ell(k, r)$ must vanish at the origin like $r^{\ell+1}$, and the real linear combination with this property is

$$v_\ell(k, r) = \frac{1}{2ik}\left[(-1)^\ell f_\ell(k, r)\mathrm{e}^{i\delta_\ell(k)} - f_\ell(-k, r)\mathrm{e}^{-i\delta_\ell(k)}\right]\,, \tag{29}$$

which for large values of r tends to

$$v_\ell(k, r) \stackrel{r\to\infty}{\longrightarrow} \frac{1}{k}\sin(kr - \tfrac{1}{2}\ell\pi + \delta_\ell(k))\,. \tag{30}$$

In the vicinity of the bound state pole we write the S-matrix

$$S_\ell(k) \equiv \mathrm{e}^{2i\delta_\ell(k)} = \frac{F_\ell(-k)}{F_\ell(k)} = \frac{(-1)^\ell\,[N_\ell G_\ell(k)]^2}{\alpha + ik}\,, \tag{31}$$

with $G_\ell(i\alpha) = 1$ and N_ℓ real.

The residue has an ℓ-dependent phase factor and we define the square root through

$$\mathrm{e}^{i\delta_\ell(k)} = \mathrm{e}^{i\pi\ell/2}\frac{N_\ell G_\ell(k)}{\sqrt{\alpha + ik}}\,. \tag{32}$$

The extra phase factor matches that in the definitions of eqs.(26) and (32) such that, with $w_\ell(k, r)$ defined as in eq.(16), the results of eqs.(17) and (18) remain unchanged with N_ℓ the asymptotic normalisation constant for angular

momentum ℓ. In particular, the bound state wave function with the asymptotic normalisation of eq.(12) is defined by

$$u_{\ell,\alpha}(r) = (-i)^{\ell} f_{\ell}(i\alpha, r) \; . \tag{33}$$

In sum, our principal result of eq.(25) remains true for arbitrary partial waves. However, in order to provide a smooth extrapolation to the bound state pole it is preferable to take out the explicit threshold behaviour by dividing by a k^{ℓ} factor to give

$$\lim_{k \to i\alpha} \left\{ \sqrt{2\alpha(\alpha^2 + k^2)} \, \left(\frac{\alpha}{k} \right)^{\ell} v_{\ell}(k, r) \right\} = -(-i)^{\ell} \, u_{\ell,\alpha}(r) \; . \tag{34}$$

Though of little importance in practical applications, this introduces an extra overall phase factor, whose origins may be traced to the definition of the partial wave solution of eq.(29).

4 Relation to the Goldberger and Watson Form

Using formal scattering theory arguments, Goldberger and Watson have derived an expression relating the normalisation of scattering and bound state wave functions [2] for the regular S-wave solution $\varphi(k,r)$, which is fixed by two real boundary conditions at the origin. The result, which depends upon the values of the Jost function and its derivative at the S-matrix pole, cannot be simplified, which means that the relation between the regular solution $\varphi(k,r)$ and the bound state wave function $u_\alpha(r)$ depends intrinsically upon the form of the potential.

The Goldberger-Watson form can however easily be recast to give a relation for the physical scattering wave function $v(k,r)$ (*cf.* eq.(11.89) of ref.[3]).

$$\lim_{k\to i\alpha}\left\{\sqrt{\frac{4i\alpha^2F(k)}{\dot{F}(k)}}\,v(k,r)\right\} = -u_\alpha(r)\,. \tag{35}$$

In the vicinity of an isolated zero the Jost function may be written as

$$F(k) = i\,\mathcal{C}(k)\,(k-i\alpha)\,, \tag{36}$$

where $\mathcal{C}(k)$ is regular and $\mathcal{C}(i\alpha)\neq 0$.

It then follows immediately that

$$\lim_{k\to i\alpha}\left\{\sqrt{\frac{4i\alpha^2\mathcal{C}(k)(k-i\alpha)}{\dot{\mathcal{C}}(k)(k-i\alpha)+\mathcal{C}(k)}}\,v(k,r)\right\} = \lim_{k\to i\alpha}\left\{\sqrt{4i\alpha^2(k-i\alpha)}\,v(k,r)\right\} = -u_\alpha(r). \tag{37}$$

At the pole this coincides with our form of eq.(25), as indeed it must, and so it is hard to understand why earlier developments [3] stopped just before the implementation of eq.(36).

However for real values of k our expression for the extrapolation function in eq.(25) remains explicitly real, whereas that of eq.(37) becomes complex. As a consequence the former provides a smoother extrapolation for the relationship between two real quantities.

To see the difference in practice, consider a one-term separable potential with shape parameter β, for which the ratio of the scattering and bound state wave

functions at the origin is given by

$$R(k) \equiv \left\{ \frac{v(k,r)}{u_\alpha(r)} \right\}_{r=0} = \frac{1+2z}{\sqrt{2\alpha(k^2+\alpha^2)}\sqrt{1+z}}\,, \tag{38}$$

where

$$z = \frac{k^2+\alpha^2}{4\beta(\alpha+\beta)}\,. \tag{39}$$

The correction terms to eq.(25) are therefore small at $r = 0$ providing k^2 and α^2 are small compared to β^2.

The extrapolation function for the Goldberger and Watson form may be easily derived from the Jost function

$$F(k) = \frac{(k-i\beta)[k+i(2\beta+\alpha)](k-i\alpha)}{(k+i\beta)[k^2+(\alpha+\beta)^2+\beta^2]}\,. \tag{40}$$

It is easily seen that this leads to large errors as soon as k^2 is comparable to α^2 and this is due to the neglect of the influence of the zero of the S-matrix at $k = -i\alpha$.

5 One-dimensional scattering

One-dimensional scattering problems show certain features which are not present in the more usual three-dimensional case [6], but our proof goes through here largely unaltered.

Assuming the potential to be an even function of the variable x, for which $V(-x) = V(x)$, it is convenient to work with even and odd solutions of the Schrödinger equation $v_+(k,x)$ and $v_-(k,x)$ which at the origin satisfy the boundary conditions

$$v'_+(k,0) = 0\,, \tag{41}$$

$$v_-(k,0) = 0\,. \tag{42}$$

For large positive values of x the functions behave like

$$v_+(k,x) \stackrel{x\to\infty}{\longrightarrow} \cos(kx+\delta_+(k))\,, \tag{43}$$

$$v_-(k,x) \stackrel{x\to\infty}{\longrightarrow} -\sin(kx+\delta_-(k))\,. \tag{44}$$

We define the normalisations of the corresponding symmetric and antisymmetric bound state wave functions through

$$\int_{-\infty}^{+\infty} dx \left[u_+^\alpha(x)\right]^2 = \int_{-\infty}^{+\infty} dx \left[u_-^\alpha(x)\right]^2 = 1\,. \tag{45}$$

With the exception of an overall $-k$ factor in eq.(44), the boundary conditions on the antisymmetric function are identical to those of the S-wave three-dimensional problem of eq.(9) combined with the vanishing at the origin. Taking into account that the normalisation integral extends down to $-\infty$ in eq.(45), one can deduce the one-dimensional extrapolation directly from the corresponding three-dimensional case in eq.(25)

$$\lim_{k\to i\alpha}\left\{\frac{1}{k}\sqrt{\alpha(\alpha^2+k^2)}\,v(k,x)\right\} = u^\alpha(x)\,. \tag{46}$$

The presence of the $1/k$ factor in eq.(46) does not upset the smoothness of the extrapolation since this is compensated by the vanishing of $v_-(k,x)$ at $k=0$,

which is a clear consequence of the antisymmetry of the function with respect to kx.

For the symmetric case we must modify the arguments given in §2. In the vicinity of a simple pole of the S-matrix, we may write

$$S_+(k) \equiv \mathrm{e}^{2i\delta_+(k)} = -\frac{2[N\,G(k)]^2}{\alpha + ik}\,, \tag{47}$$

where $G(k)$ is analytic in the neighbourhood of the pole and is normalised there to $G(i\alpha) = 1$.

Now it is known that as $k \to 0$, $\delta_+(k) \to \pi/2$ unless there is a zero-energy bound state [6]. This is one of the special features of one-dimensional scattering, which causes the one-dimensional transmission coefficient to vanish at zero energy. When this condition is imposed upon eq.(47), it follows that

$$G(0) = \frac{1}{N}\sqrt{\frac{\alpha}{2}}\,. \tag{48}$$

Due to the symmetry of the problem, we need only consider the region $x \geq 0$, and there the Jost solution is defined by its asymptotic behaviour

$$f(k,x) \;\stackrel{x\to\infty}{\longrightarrow}\; \mathrm{e}^{ikx}\,. \tag{49}$$

This allows the even function to be written as

$$v(k,x) = \frac{1}{2}\left[f(k,x)\,\mathrm{e}^{i\delta_+(k)} + f(-k,x)\,\mathrm{e}^{-i\delta_+(k)}\right]\,. \tag{50}$$

After defining a non-normalised bound state wave function $u_+(x)$ with a large-x limit of $\mathrm{e}^{-\alpha x}$, as in eq.(12), all the subsequent manipulations follow as in the three-dimensional proof. This is because in the symmetric case the derivatives of the wave functions vanish at the origin, and so it is still permissable to discard the left hand side of eq.(15) at $x = 0$ to leave, as before,

$$u'_+(x)v_+(k,x) - u_+(x)v'_+(k,x) = (\alpha^2 + k^2)\int_0^x \mathrm{d}x' u_+(x')v_+(k,x')\,. \tag{51}$$

It is then straightforward to show that the one-dimensional result of eq.(46) is valid for both symmetric and antisymmetric wave functions.

6 Conclusions

We have given a simple proof of the relation between the normalisations of the bound and scattering wave functions at the bound state pole which is on a par with the standard proof of the effective range expansion [1]. Apart from being formally correct, the result is useful in practice because the extrapolation function is smooth in k^2. As we saw in the case of the separable potential in §3, corrections to it only become important when $1/k$ is of the order of the range of the potential. It is therefore possible to use the theorem to form approximations for scattering wave functions in terms of that of the bound state. For the S-wave Paris neutron-proton triplet potential [7] such an approach is reliable out to radii of 1.7 fm for centre-of-mass energies up to at least 20 MeV [8].

Already in 1952, Watson [9] used such arguments to estimate the final state interaction effects in $pp \to \pi^+(pn)$ at low excitation energies in terms of the cross section for $pp \to \pi^+ d$. The relative scattering/bound state normalisation was there established as an *approximation* using effective range theory, though in practice it differs little from our result at the pole. Providing the momentum transfer is large, as it is for pion production, then the corresponding transition operator is sensitive to the short range part of the neutron-proton wave function where our theorem provides a valid approximation. In addition to providing a useful description of $pp \to \pi^+(pn)$ data near threshold and at higher energies, it allows one to understand quantitatively the final state interaction regions in $pn \to \eta(pn)$, $pd \to \pi^0(pd)$, and $dp \to p(pn)$ at high momentum transfers [4, 8, 10].

The extension to higher partial waves described in §3 is likely to be of less significance since it is harder to investigate the effects of P-wave final state interactions unless the S-wave is suppressed. Nevertheless the modifications to our principal result of eq.(25), engendered by threshold kinematic factors for $\ell \neq 0$, are of importance here.

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